An application of C-algebras to quantum statistical mechanics of systems in equilibrium

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INTRODUCTION AND SUMMARY

The aim of Statistical Mechanics is to derive the properties of macroscopic systems from the properties of the individual particles and their interactions. In particular it is the task of Statistical Mechanics to give an explanation of phase transitions, transport phenomena and the approach to equilibrium in the course of time for a non-equilibrium system.

Although, in certain models, one can prove the existence of a phase transition - for instance in the Ising model in two and more dimensions with zero external field - theoretically the situation with respect to phase transitions in general is not well understood.

Much the same holds for transport phenomena and the approach to equilibrium. All attempts to derive a transport equation of the Boltzmann type for a non-dilute gas have failed up to now. Although one can formally derive such an equation [1], its meaning is not clear. In particular the transport coefficients - for instance the viscosity - that one derives from such an equation should, for low densities, approach those derived from the Boltzmann equation for a dilute gas. However, if one makes a density expansion for the transport coefficients, the first order correction term tends to infinity for large times [2].

These remarks suffice to show that several of the basic problems in Statistical Mechanics are as yet unsolved.

In an attempt to bring these problems to a solution new methods have been developped. One of these methods, the algebraic approach [3], [4], [5], and more specifically the approach in terms of C^*-algebras and their representations, will be used in this thesis to discuss properties of states in thermal equilibrium. Before embarking in this subject let us discuss some of the main reasons why one is always interested in infinite systems, i.e. systems which are infinitely extended and have infinitely many degrees of freedom.

As mentioned above, macroscopic systems are the objects of study in Statistical Mechanics. Macroscopic systems are composed of a large number of particles. In simple cases macroscopic systems consist of a small number of components. To approximate such a large system by an infinite system is on the one hand a very good approximation and on the other hand leads to a considerable simplification.

There is, however, a more fundamental reason for dealing with infinite systems. Most of the phenomena which are typical for macroscopic systems can be given a precise mathematical formulation only in the thermodynamic limit. According to a famous theorem of Poincaré any finite system will return to its initial state after a sufficiently long time, the Poincaré cycle. It has also been shown [6] that a p-v diagram of a finite system of identical particles must have a continuous derivative, and therefore does not exhibit a phase transition.

Whereas both in conventional Statistical Mechanics and in the C^*-algebra approach one deals with infinite systems, there is an essential difference in the procedure. To point out this difference we shall briefly review the conventional method. In the conventional theory one deals initially with a finite system, with particle number N and volume V. The state of the system is defined by a density operator ρ. The average value $\langle A \rangle$ of an observable A is then given by the following expression

$$\langle A \rangle = \mathrm{Tr}\rho A / \mathrm{Tr}\rho. \tag{1}$$

For an equilibrium state one uses, according to Gibbs, the density operator

$$\rho = \exp\left[-\beta(H-\mu N)\right] \tag{2}$$

where H is the Hamiltonian of the system, N the particle number operator, $\beta = (KT)^{-1}$ and μ is the chemical potential. It is well-known that, although the thermodynamic limit of this density operator does not exist, the average $\langle A \rangle$ will have a limit under suitable conditions. This limit gives the average value of A for the infinite system. It is clear from this procedure that it is unavoidable in this approach to start always with a finite system and to take the thermodynamic limit afterwards.

In the C^*-algebra approach one treats infinite systems from the very beginning. This approach is a generalization of the well-known Field-theoretical treatment of Quantum Statistical Mechanics in terms of Green's functions. Let us therefore briefly review the Green's function method in Quantum Field theory.

In a Quantum Field theory one considers an infinite number of pairs of canonical variables, represented by operators - on a suitably chosen Hilbert space. Perhaps the simplest representation space is the one known as Fock space. In this space one has a no-particle state from which the one-, two-,

... particle states can be constructed by applying suitably chosen combinations of the field operators, i.e. creation operators. The Green's functions for non zero-temperature are expectation values of field operators and their products computed in the Grand-Canonical ensemble.

It is known that infinite quantum systems cannot be treated effectively in Fock space. For instance, if one tries to calculate the ground state wave function, in Fock space, for the weakly interacting Fermi-gas in the thermodynamic limit, one obtains meaningless expressions [7]. This result is obtained in perturbation theory. This is a general feature, however, of quantum systems with an infinite number of degrees of freedom [8], [9], [10].

The conclusion to be drawn from this is that thermodynamic ground-state averages of field operators and their products, i.e. zero-temperature thermodynamic Green's functions, cannot be reproduced as expectation values computed by means of a vector in Fock-space. As already indicated, non-zero temperature Green's functions for infinite systems cannot be defined by means of a density operator on Fock space.

The Green's functions as functionals over the algebra of field operators define a natural Hilbert space, and a corresponding representation of the field operators, which can be explicitly constructed. In this Hilbert space the Green's functions are then reproduced by expectation values computed by means of a vector.

Instead of the field operators we shall discuss a C^*-algebra $\mathfrak{A}$ on Fock space, which is suitably constructed from the field operators for systems contained in finite regions. This algebra $\mathfrak{A}$ is called the algebra of quasi-local observables. Its local structure represents the local nature of any measurement or disturbance the physical system can undergo and which is at the experimentalist's control [4].

The role of the Green's functions is then taken over by positive linear functionals (states) over the C^*-algebra $\mathfrak{A}$. We shall discuss such states describing infinite quantum systems in thermal equilibrium and investigate some of their properties in their natural representation, which also in this case can be explicitly constructed.

Conventionally in the Green's function method, the dynamics - as any other symmetry group, such as translations in space and gauge transformations - induces, in the Heisenberg picture, a group of transformations of the field operators. In the algebraic approach their part is filled by groups of automorphisms of the algebra $\mathfrak{A}$. One can then describe the invariance - or lack of invariance - of the physical system under consideration in terms of the response of the state to such an automorphism. In particular this shows whether a system exhibits a certain symmetry or that the symmetry is broken [5].

As already mentioned, for a finite system, an equilibrium state as prescribed by the Grand Canonical ensemble is characterized a density operator ρ. Due to the invariance of the right-handside of (1) for cyclic permutations of its arguments one derives an interesting analyticity property of $\langle A_t B\rangle$ as a function of complex t, known as the Kubo-Martin-Schwinger boundary condition [12], [13]. (Here A_t denotes the time translated observable A). The K.M.S. boundary condition is a powerful calculational tool in the conventional theory of Green's functions [14].

For infinite quantum systems the density operator ρ does not exist, and therefore the validity of the K.M.S. boundary condition is not a priori guaranteed for a state describing an infinite system.

However, for states of infinite systems that are obtained from states of finite systems by taking the thermodynamic limit, it can be shown that the K.M.S. condition still holds [11].

Independent of the way in which we have obtained the state of the infinite system, we shall investigate some further properties of the K.M.S. boundary condition. We are then continuing the analysis given in [11].

In chapter I we discuss first (section 1) the algebraic treatment of an n-particle system together with some general properties of a C^*-algebra. In section 2 the algebra $\mathfrak{A}$ and its states are discussed. In section 3, the case of a system enclosed in a box is treated, whereas in section 4 we give the K.M.S. boundary condition for a system in a box V.

In chapter II the role of the dynamics is discussed (section 1), in particular the conditions under which the dynamics induces a group of automorphisms of $\mathfrak{A}$. In section 2 we give a brief discussion of the thermodynamic limit and of the consequences of the K.M.S. condition for the infinite system.

In chapter III the uniqueness of some of the consequences of the K.M.S. condition is discussed (section 1 and 2). In section 3 we give the relevant properties of a Quasi-Unitary algebra along with the proof that the representation of $\mathfrak{A}$ given by a K.M.S. state is the left-ring of a Quasi-Unitary algebra. In section 4 we investigate to what extent a cyclic and separating vector, for the von Neumann algebra in the representation space, can replace the K.M.S. condition.

Chapter IV section 1 describes the physical properties of states giving rise to a factor representation of type III. In particular their relative insensitivity for local disturbances is discussed. Such states are called physically pure.

The rest of chapter IV is devoted to a decomposition of an arbitrary K.M.S. state into physically pure states. Moreover this decomposition is compared with the known decomposition into extremal invariant states with respect to space translations. Concerning the latter, similar results were obtained in [15].